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LCA AND CHEMISTRY

# A methodological improvement for assessing petrochemical projects through life cycle assessment and eco-costs

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**Abstract**
*Purpose* As the debate on how to effectively link life cycle analysis (LCA) and negative externalities of the products or processes is still unsolved, an improved methodology that involves the private and social (environment) profitability to petrochemical projects in Mexico is presented. We incorporate both environmental impacts, identified through the LCA, using the eco-costs model, within a project appraisal analysis. The eco-costs are a single LCA-based indicator of environmental burden, based on the concept of marginal prevention costs, i.e. costs required to bring back the environmental degradation to a sustainable level.
*Methods* The methodology was carried out in four steps. First, the potential environmental impacts (in physical units) were assessed through life-cycle assessment. Second, the marginal prevention costs of pollution (eco-costs) of impact categories were estimated. Third, since these monetary values are given for a European income level, eco-costs were adjusted to Mexican income levels (i.e., benefit transfer). Fourth, these adjusted values were used for assessing the financial viability of two petrochemical projects at two stages of installed capacity.
*Results and discussion* The costs of marginal prevention (eco-costs) changed from 1.62 USD/kg of acrylonitrile in the old design to 0.926 USD/kg in the redesign. In case of vinyl chloride monomer (VCM), the eco-costs were from 16.08 USD/kg of VCM for the stage design to 1.62 USD/kg for the operational stage (ex post). The sensitivity analysis identified that only 15 % of these eco-costs, in the case of acrylonitrile, and 1.5 % for the VCM, could be incorporated to the costs of the project without affecting the profit on the investment.
*Conclusions* The developed methodology was helpful to express potential environmental impacts in monetary units as financial indicators in a project appraisal. Thus, the methodology can be used to internalize the eco-costs into product prices, shifting the financial burden to firms and consumers, in order to offset the high costs of the green net national product.

**Keywords** Benefit transfer · Eco-costs · Project appraisal · Petrochemical industry · Mexico · Acrylonitrile · Vinyl chloride monomer

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## 1 Introduction

A number of chemical substances used in the life cycle of a product are harmful to both ecosystems and living beings if released into the environment (Huijbregts et al. 2000). Effects, in addition to acute and immediate harm, may induce cancer, mutations, reproduction harm, birth handicaps, or dysfunction of the endocrine system (Kuczenski et al. 2011). Many of such

impacts (both environmental and in human health) are observed in the petrochemical industry (Yu et al. 2006; Axelsson et al. 2010; Al-Jabri and Baawain 2011). For example, in the production of acrylonitrile in Mexico, high concentration of hazardous substances as cyanide may be discharged (<40 mg/l) in the wastewater, causing negative effects on the enzymatic processes and interrupting the cellular respiration, reducing the carbonaceous matter removal and the processes of nitrification and denitrification in activated sludge reactors (Morales-Mora et al. 2012b). Neurobehavioral effects of occupational exposure to acrylonitrile have been documented in Chinese workers (Rongzhu et al. 2005). Furthermore, a recently assessment in 2012 with leak detection and repair at the volatile organic compounds (VOC) emission at the vinyl chloride monomer (VCM) Mexican plant showed nine leaks in valves of VCM in concentrations of 1,000 and 1,2-dichloroethane higher than 100,000 ppmv. Environmental impact as a result of the dichloroethane and vinyl chlorine monomer (EDC/VCM) process several chlorinated hydrocarbon byproducts are formed (UNEP 2005). It is generally recognized that dioxins can be formed during the production of EDC by oxychlorination (PE-EuropeGmbH 2004). In the same way, increased risk of lung cancer has been reported in workers occupationally exposed to VCM (Scléo et al. 2004; Gennaro et al. 2008).

In economics, these negative effects represent an unaccounted external cost (i.e., negative externality) since the action on an agent results in uncompensated welfare losses for third parties. For example, Jantzen and Pesic (2004) report that environmental costs may amount up to 2.4 % of the gross domestic product (GDP) in The Netherlands and from 4.7 to 14.7 % in Serbia. In China, the air pollution impacted on the GDP in 3.8 % in 2003 (Heck and Hirschberg 2011). In the European Union, the damage caused by air pollution to human health was estimated in 300,000 premature deaths per year and external costs of €120 billion per year by electricity and transport (Di Valdalbero and Valette 2010).

In the case of Mexico, due to the deficiencies in monitoring and regulating of environmental performance for industrial activities, the environmental costs were 7.9 % of the GDP in 2009 where the mining sector (oil) contributed with the 19 % of the total those costs (INEGI 2011). However, only 14.2 % of the environmental protection budget was directed to reducing the effects produced by environmental pollution. Environmental costs are even higher where the oil petroleum and petrochemical industry are located, representing a major area of concern because of a reduced budget for environmental prevention and because the oil production is high. In fact, Mexico is the ninth largest oil producer in the world (SENER 2013).

For example, the industrial port of Coatzacoalcos, in SE Mexico, registers a strong industrial oil, gas, and petrochemical activity (PEMEX 2009). In this zone, the flows of degraded materials, energy, and pollution have been discharged into the water, air, and soil, causing major impacts to the local population (Perez-Zapata et al. 1982; INE 2010) and aquatic fauna (INE 2007; Ruelas-Inzunza et al. 2007; Ruelas-Inzunza et al. 2009; Espinosa-Reyes et al. 2009; Gonzalez-Mille et al. 2010).

In particular, the petrochemical industry is of paramount importance from both the economics and environmental point of view. In spite of this, few studies have been conducted through life cycle analysis (LCA) in the petrochemical industry (e.g., Kawauchi and Rausand 1999; Lee et al. 2009; Portha et al. 2010a,b; Al-Salem et al. 2012; LaRosa et al. 2013), but none of these have assessed the costs of their environmental impacts (Morales-Mora et al. 2012a).

A recent survey presented by the World Bank (2009) for the oil and gas sector of 29 oil-producing countries concluded that the environmental impact assessment is still used for the evaluation of projects with emphasis in the approval in its final phase for the permission from the environmental authority. In contrast, there is no focus on LCA for minimizing the environmental impacts from the initial phase of project planning, which is the stage where changes in design and use of end of life can be made (World Bank 2009; Manuilova et al. 2009). Indeed, when analyzing costs in LCA, the most critical phase is design, according to Korpi and Ala-Risku (2008), given that about 70–90 % of costs are defined at this stage.

During the past years, there have been efforts to incorporate environmental costs to the products, procedures and services through LCA (e.g., Saling et al. 2007; Hong et al. 2009). Yet, there is no methodological consensus (or the mechanism has not been clear) for assigning economic values to the categories of impact (Guinée et al. 2004; Korpi and Ala-Risku 2008; Settanni 2008). Furthermore, it has not been defined how to incorporate this value to products, procedures, and services of the LCA as a prevention tool of the environmental impacts nor in the financial analysis of actual projects. These tools would help to either reject or accept projects with a sustainability focus. According to Zhang et al. (2010), the use of LCA in a conventional manner might even result in decisions that would result in potential degradation of ecosystem services.

Vogtländer et al. (2010) have developed and integral method to evaluate the environmental impact and its relationship to the market value of a product using LCA and is called the eco-costs/value ratio (EVR) model. Eco-costs are the costs that should be spent to reduce the environmental pollution and material depletion in our economy, avoiding to reach the carrying capacity of Earth (the so-called "no-affect level"). According to Vogtländer et al. (2010) eco-costs are "neglected or hidden obligations" since they are not accounted for in the real costs of actual production chains. These eco-costs have been estimated on the basis of technical measures to prevent pollution and depletion of materials and energy to a level, which is sufficient to make our society sustainable (Vogtländer and Bijma 2000; Vogtländer et al. 2010, 2001;Mestre and Vogtlander 2013).

Accounting for both eco-costs and externalities has gained interest for decision making in emergent economies (e.g., Guse et al. 2011). However, the lack of reliable information to obtain accurate estimation of eco-costs remains a major challenge to solve. In LCA and economics, cost allocation problems must be considered because they become liable to pay for the consumption of goods and services (Ciroth 2009).

Although cost analysis in LCA deserves further attention, the lack of reliable data is a major obstacle. Hence, further methodological alternatives are needed for coping with this urgent matter but, at the same time, keeping with high quality standards in cost estimates (Ciroth 2009). In many cases, such estimations are preliminary results, which could give a benchmark or baseline for further more refined estimates.

In Mexico, there are no studies related to the estimation of the environmental costs of the oil, gas, and petroleum industry, where the direct and indirect environmental costs are incorporated into the products and services prices. Therefore, it is urgent to develop an approach where those costs are considered and evaluated to prevent, stop, or mitigate the effects on the environment caused by the oil petroleum industry activities, in particular, and other social activities, in general. This allows applying sustainable politics in the country.

As a solution, benefit transfer (BT) is a method that involves the use of research results from preexisting primary studies at one or more sites or contexts to predict welfare estimates such as willingness to pay or related information for other sites or contexts (Brookshire and Neill 1992; Desvousges et al. 1998; Wilson and Hoehn 2006; Liu et al. 2011; Rosenberger and Johnston 2013). This method is known as BT. Its main advantages are its low cost, if the information of the value known of other good is precise and adjusted, and high reliability, if correctly applied (Jantzen and Pesic 2004).

Hence, the aim of this paper is to present an improved methodology (previously presented in Morales-Mora et al. 2012a) that involves the private and social (environment) profitability to Mexican petrochemical projects. Environmental impacts, identified through the LCA, and the estimation of the costs of marginal prevention with the models of eco-cost are incorporated by means of BT. The methodology was applied in two petrochemical projects as study cases: the acrylonitrile and vinyl chlorine monomer (VCM) processes (Figs. 1 and 2, respectively).

## 2 Methodology

### 2.1 Life cycle assessment, eco-costs, and benefit transfer approaches

The present study follows the methodology shown in Fig. 3, which consists of six phases that combine LCA and the economic analysis through eco-costs model for project appraisal. Morales-Mora et al. (2012a) described this methodology, but neither eco-costs adjustment for Mexico nor its use for evaluation from the project phase was performed. Therefore, it was improved in the present study by: (1) providing major information on the inputs at every stage; (2) defining a mechanism to adjust economic values from the eco-cost database (Vogtländer et al. 2010), through the benefit transfer method; and (3) incorporating a sensitivity analysis in the phase of economic evaluation to identify the percentage of the eco-costs in the financial project analysis.

The LCA was performed according to the ISO 14040 standard procedure (ISO 2006) with the SimaPro software, using PEMEX-PETROQUIMICA own database (for a detailed description see: Morales-Mora et al. 2012a). Impacts were assessed with the ReCiPe method (Goedkoop et al. 2009). The costs of the target scenarios were assessed using the eco-costs method (Vogtländer et al. 2010) in four steps. In the first step, the marginal prevention costs during the life cycle ("cradle to grave as well as cradle to cradle") for toxic emissions, material depletion, energy consumption, and conversion of land were calculated (Vogtländer et al. 2002, 2010). In the second step, the method of BT was used to adjust the values obtained from the eco-costs database (see Section 2.2. below) in order to adapt them to the Mexican context (Brouwer and Spaninks 1999; Wilson and Hoehn 2006). It was assumed that the Delft Technology University database (Vogtländer et al. 2010) on eco-costs fulfill the remarks of Ciroth (2009) with respect to data quality. In the third step, in order to estimate the economic resources, which must be directed to preventing or reversing the deterioration of the environmental services offered by ecosystems and demonstrate its use in the evaluation phase of projects, two cases studies of petrochemical projects in Mexico were performed. In the last step, a project appraisal analysis with these data was applied.

The steps of integration of LCA and eco-costs (Fig. 3) are described in detail in the next section.

#### *2.1.1 Goal and scope definition for two case studies*

The goal of this study was to improve the LCA methodology of Morales-Mora et al. (2012a) to measure and quantify the potential environmental impacts (in physical units), estimate the eco-costs, and transform them into economic units of a petrochemical project. Using eco-costs (such as pollution prevention and depletion of materials), a project appraisal was carried out in terms of net present value (NPV) and internal rate of return (IRR) for the acrylonitrile and VCM petrochemical processes. To either accept or reject the proposal based on the eco-costs, two scenarios for each process (Table 1) were evaluated:

(a) The acrylonitrile old plant's operative performance of 50, 000 tons/year of incinerated by-products and the current

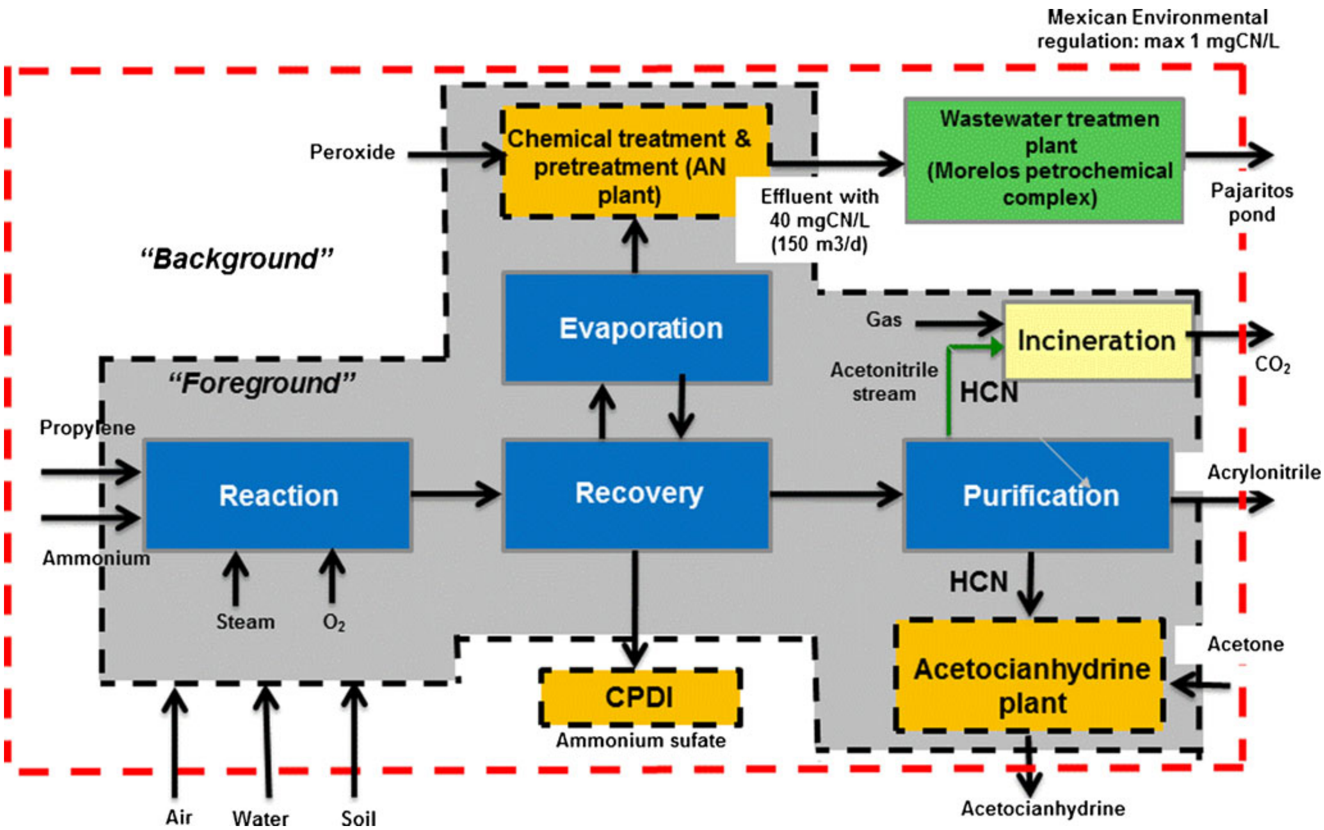



**Fig. 1** Acrylonitrile plant flow diagram from Morelos Petrochemical Complex, Mexico (after Morales-Mora et al. 2012a,b)

operation of 60,000 tons/year using the by-products, where the waste stream is treated in order to generate profitable products (Fig. 1).

(b) The VCM redesign (in 2004) with an enlarged capacity of 405,000 tons/year versus the operational conditions of the plant after (ex post) the redesign (in 2009). This plant has been operated postenlargement, with a factor of service below the original project's target, as well as high-energy consumption, materials, water, and generation of chlorinated organic compounds above the projected level (Fig. 2).

### 2.1.2 Functional unit

The functional unit (FU) was defined as the production of 1 kg/day for both products because the value used

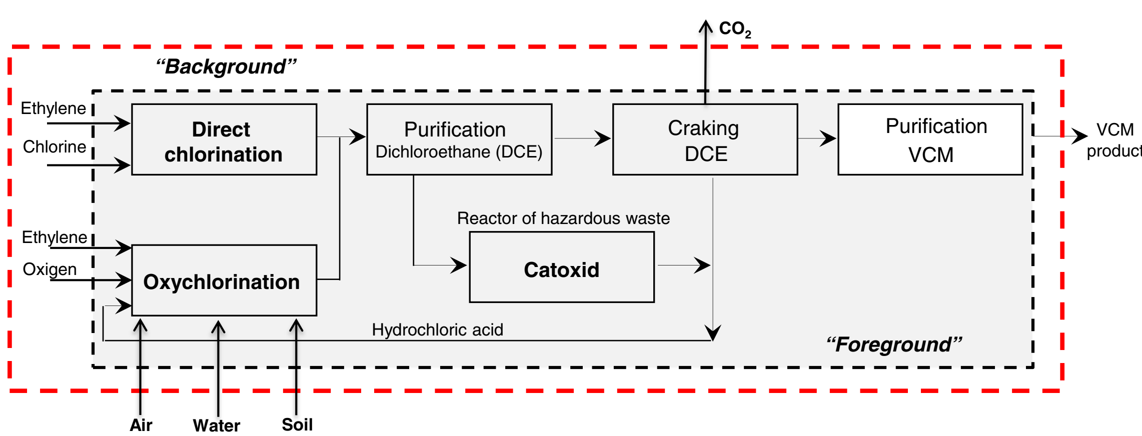



**Fig. 2** Production process of the VCM plant from Pajaritos Petrochemical Complex

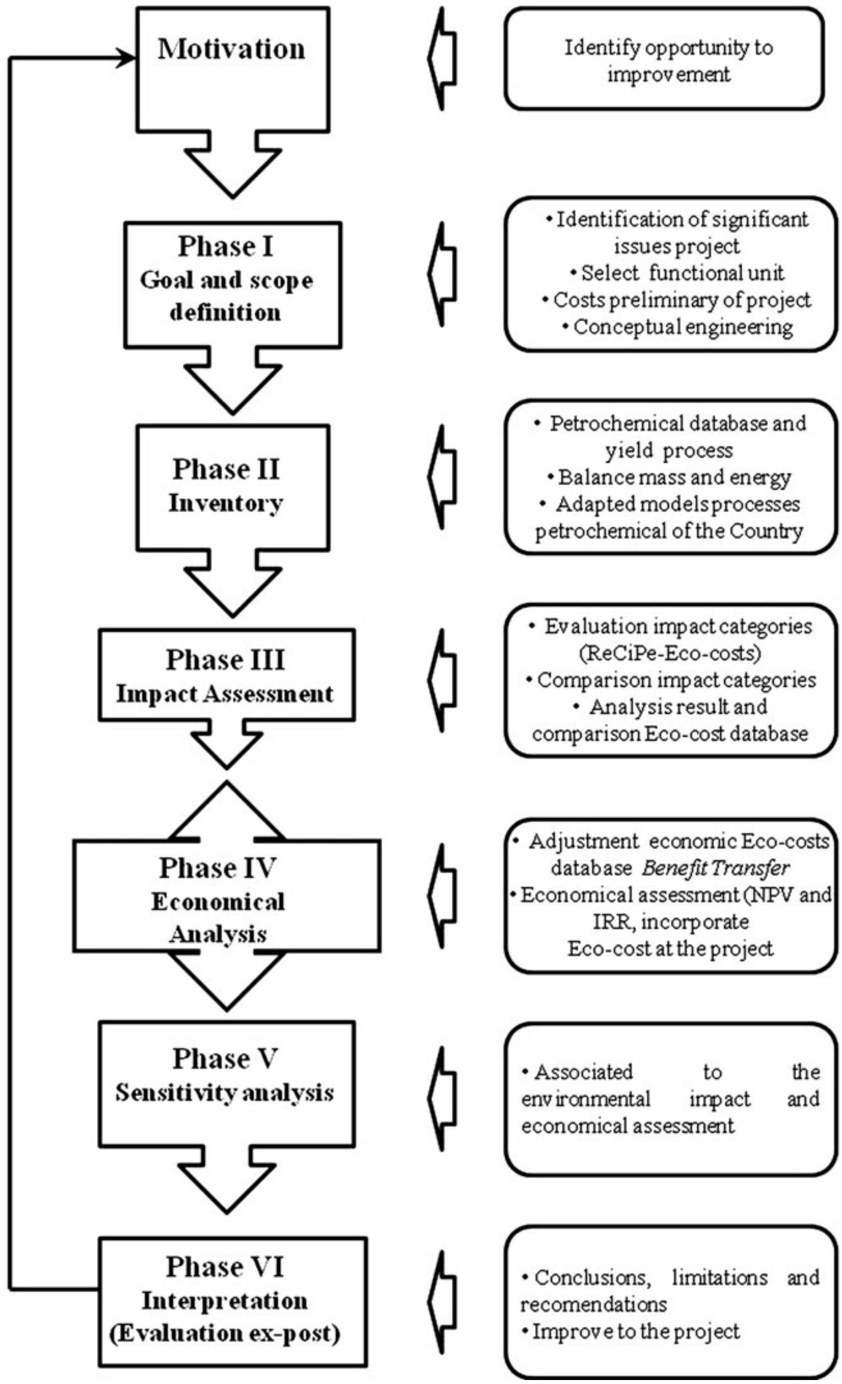



**Fig. 3** Flow chart showing the integration of LCA and Eco-costs (after Morales-Mora et al. 2012a,b)

of the eco-costs database is expressed simply as €/kg (see www.ecocostsvalue.com/). The price of the petrochemical product, usually expressed in tons, was aligned to this FU.

*2.1.3 System boundaries*

System boundaries and flow diagrams of both plants are shown in Fig. 1 (the acrylonitrile case) and Fig. 2 (VCM case at Pajaritos Petrochemical Complex). Such diagrams show the main types of raw material and emissions to the environment throughout the life cycle and help to identify possible ways to achieve environmental improvements, particularly in the redesigned plant.

A model based on the expansion system of Weidema (1999) and, according to JRC (2010), was used for multi output processes in order to avoid allocation. The transport

**Table 1** Scenarios evaluated for two case studies

| Products | Scenario A | Scenario B |
|---|---|---|
| Vinyl chlorine monomer | Redesign: 200,000–405,000 tons/year (direct chlorination and oxychlorination)<br>Data: 2004 | Operation later (ex post) to the redesign<br>405,000 tons/year<br>Data: 2009 |
| Acrylonitrile | Old design 50,000 tons/year<br>Data: 2005 | Redesign 60,000 tons/year<br>Data: (November–December 2009) |

and product use phases are outside the system boundaries for both case studies because PEMEX-PETROQUIMICA delivered free on board their products.

### 2.1.4 Inventory

We used the gross inventory to produce 1 kg of acrylonitrile for each scenario as reported by Morales-Mora et al. (2012a). In the case of VCM, the inventory is shown in Table 2. Data were obtained from direct measurements, while the annual averages are indicated in Table 1 from the PEMEX-PETROQUIMICA database.

### 2.1.5 Life cycle impact assessment and eco-costs

The life cycle impact assessment (LCIA) was performed using the ReCiPe method (Goedkoop et al. 2009) including 18 environmental midpoint categories and three endpoint categories, which is the same used to model of eco-costs.

The results of the midpoint categories obtained with ReCiPe and Simapro 7.2.3 were combined with the referent cost acrylonitrile and VCM from Eco-costs database (www.ecocostsvalue.com/index.html) to carry out the LCA. The eco-costs for both scenarios were calculated by linear interpolation from the results of the LCIA and then were compared with eco-costs database (Morales-Mora et al. 2012a), in order to obtain the eco-costs for the study cases. The calculation structure of the eco-costs system was carried out as in the study of the model of the EVR (http://www.ecocostsvalue.com/EVR/model/theory/subject/8-LCA.html).

## 2.2 Economic analysis: adjustment of economic values

When a BT is carried out for countries with different income levels, it is important to adjust the purchasing power parity (PPP) of both countries, emphasizing the influence of price level differences between the original and the current study (Brouwer and Spaninks 1999; Rosemberg and Loomis 2003; Wilson and Hoehn 2006). The exchange rates are used to compare data from the original studies in the current study (Ready et al. 1999). This is done by defining a basket of products and services, then calculate the total local/national costs for that basket, and then compare these costs for different countries (Jantzen and Pesic 2004).

Hence, the economic value of the marginal prevention costs from The Netherlands database eco-costs (Vogtländer et al. 2010) was adjusted to the Mexican context. It is important to

**Table 2** Gross inventory to produce 1 kg/day of vinyl chloride monomer (VCM) for each scenario

| Inventory | Unit | VCM 2004 Scenario A | VCM 2009 Scenario B |
|---|---|---|---|
| Avoided load | | | |
| Hydrochloric acid 30 % in water (by-product) | kg | 0.0267 | 0.5954 |
| Inventory (input) | | | |
| Raw material, energy, and water | | | |
| Ethylene | kg | 0.4920 | 0.5449 |
| Chlorine | kg | 0.5673 | 0.7568 |
| Oxygen | kg | 0.1736 | 0.0915 |
| HCI | kg | 0.6150 | 0.5942 |
| Liquid nitrogen | kg | 0.0211 | 0.1494 |
| Cooling water | kg | 333.60 | 940.14 |
| Water | kg | 1.960 | 0.0 |
| Caustic soda | kg | 0.04825 | 0.3070 |
| Steam | kg | 0.5500 | 2.591 |
| Electricity | kWh | 47.30 | 91.75 |
| Natural gas | kg | 0.0784 | 0.0922 |
| Output | | | |
| VCM | kg | 1 | 1 |
| Emissions to air | | | |
| VOC's | kg | 0.0004 | 0.6045 |
| Emissions to water | | | |
| $BOD_5$ | kg | 1.2800 | 1.2800 |
| COD | kg | 5.8799 | 5.8799 |
| 1,2-Dichloroethane (EDC) | kg | 0.0 | 0.678 |
| Emissions to soil | | | |
| Industrial waste | kg | 0.0022 | 0.0022 |
| Sludge with EDC | kg | 0.0054 | 0.0054 |
| Sludge oil | kg | 0.00003 | 0.00003 |
| Waste and emissions to treatment | | | |
| Wastewater to treatment plan | liters | 13.04 | 13.04 |

outline that the petrochemical processes conditions in both counties are similar because they present the same technology, raw materials, inputs and product, among other factors, so it is possible to use The Netherlands context in the current study. Therefore, the BT methodology is valid to estimate (King et al. 2004) eco-costs for Mexico. The detailed adjustment procedure is shown in Fig. 4. The first step is to make the correction of economic parameters (e.g., PPP). To adjust the eco-costs for 2007 to the present (i.e., 2011), the Mexican producers price index (Banxico 2011) was used. The percentage of deflation from June 2007 to May 2011 was 18.04 %. In addition, Eq. 1 was applied (Bateman et al. 2002):

$$a_i = \left(Y_i/Y_j\right)^e \quad (1)$$

where $a_i$=PPP, $Y_i$=per capita income in Mexico, $Y_j$=per capita income of the country of origin (The Netherlands), and $e$=income elasticity of demand to improve the environment, which is inelastic ($e$=0.35). Table 3 shows the values used in this work.

The income elasticity of demand was used adopting the value proposed by Gonzalez-Martinez (2001) for Mexico. Then, the $a_i$ was obtained as shown in Eq. 2:

$$a_i = (13,800/40,500)0.35 = 8.08 \quad (2)$$

A flow chart for adjusting the eco-costs (The Netherlands) by inflation, PPP, and elasticity for Mexico, applied benefit transfer approach is presented in Fig. 4.

Then, the total correction factor (deflation, PPP, and elasticity) for the total eco-costs was 26.48 %, which was incorporated for obtaining the marginal costs of the eight impact categories (LCIA) in the eco-costs database (Vogtländer et al. 2010) for both scenarios, obtaining the adjusted values to Mexico.

Finally, an economic evaluation was carried out using the production volumes, the consumption of raw material, services, prices, incomes, costs (i.e., eco-costs already adjusted to Mexico), revenues, and investment. Based on this information, two financial indicators (i.e., NPV and IRR) were employed (Blank et al. 2005). A discount rate of 12 %, a tax rate of 30 %, and $12.90 MX pesos/USD exchange rate, were considered.

**Table. 3** Values of gross domestic product (GDP) and PPP used in the benefit transfer method

| Country | GDP (PPP-2010) USD$ (billion) | GDP per capita (PPP-2010) (USD[a] $) | PIB as % the GDP |
|---|---|---|---|
| Mexico | 1.56 | 13,800 | 34 |
| The Netherlands | 600.4 | 40,500 | 100 |

[a]Exchange rate $11.72 MxM by 1 USD (as for 11-07-2011)

## 2.3 Sensitivity analysis (economic and environmental)

A sensitivity analysis (SA) was performed to identify key variables that had a major influence on the economic results of the project, as well as the decrease of incomes due to the increase of costs, under each scenario.

Due to the fact that total eco-costs (USD/kg of product) may represent a high cost in the sale price of one kg of petrochemical product, variables fluctuated within a predetermined rank for estimating a wanted level of NPV in our sensitivity analysis.

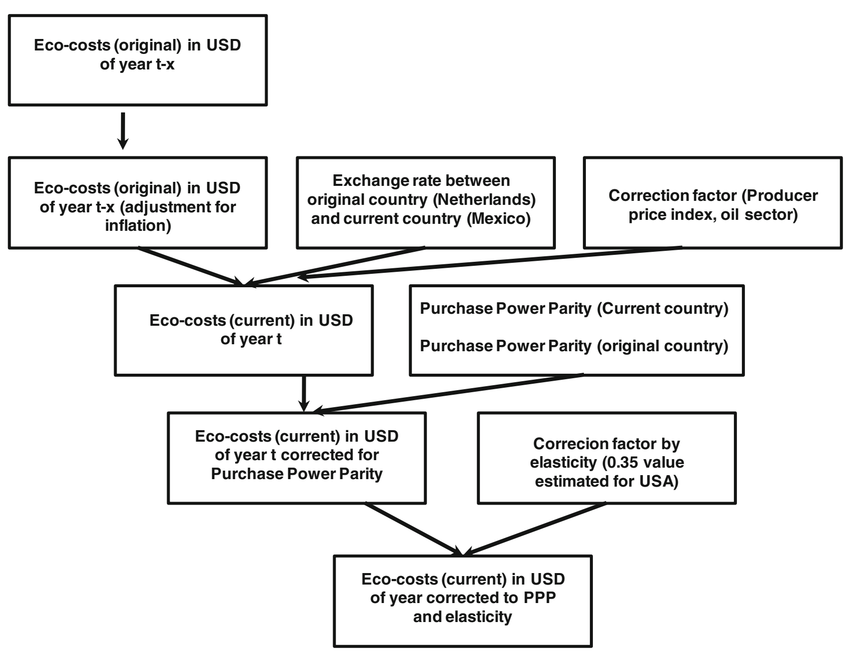



**Fig. 4** Diagram of the detailed adjustment procedure of purchasing power parity (PPP) to correct the eco-cost economic values (adapted from Jantzen and Pesic 2004)

Variables fluctuated one by one in the estimated rank in order to recognize how the NPV behaves when the eco-costs change, while time, prices, quantities, and other variables remained constant. This allowed us to find the percentage which was suitable for incorporating eco-costs without affecting the profitability of the project (Blank et al. 2005; Morales-Mora et al. 2012a).

The results from the sensitivity analysis, associated to environmental impact, were reported as sensitivity ratios for each combination of input parameter and impact category. The Monte Carlo method was chosen as stochastic simulation model to characterize the sensitivity of the LCIA results (Guinée 2002).The SA associated to the environmental impact for both processes were estimated using the SimaPro software.

## 3 Results and discussion

### 3.1 Life cycle impact assessment

#### *3.1.1 Acrylonitrile case study*

In previous study (Morales-Mora et al. 2012a), a LCA impact assessment was performed for these processes; however, the eco-costs were not adjusted for Mexican conditions, drawback corrected in this work. In order to facilitate comparison between the projects assessed in the present study, Table 4 recalls the results of a previous study where the value of eco-costs was not adjusted to Mexico. The environmental impacts of the acrylonitrile redesign showed higher impacts (freshwater ecotoxicity, marine ecotoxicity, and urban land occupation) than the former plant. The prediction of the impact of the first two categories is supported by a previous study (Morales-Mora et al. 2012b), where it was reported that high concentration of hazardous substances as cyanide in the wastewater could have caused negative effects on the cell that reduced the carbonaceous matter removal and the processes of nitrification and denitrification in activated sludge.

However, the redesign showed an overall improvement in environmental performance with a reduction in 11 of the 18 impact categories assessed and 36 % in the global impacts. The results obtained in the damage categories, showed that the percentage of reduction was 31.2 % in the redesign. In a previous study (Morales-Mora et al. 2012a), it was demonstrated that the human health endpoint category presented the highest reduction (48.4 %). Still, despite this significant reduction, health effects due to the occupational exposure to acrylonitrile remain as a potential hazard, as in the case, for instance, of Chinese workers (Rongzhu et al. 2005). This means that health effects cannot be explained with LCA human toxicity results due to the missing step of risk and exposure measurement and due to the differences of mid- and end-term indicators. Moreover, in the same study

**Table. 4** Percentage reduction of the environmental impacts in midpoint categories (Morales-Mora et al. 2012a)

| Impact category | Unit | Acrylonitrile old design (A) | Acrylonitrile redesign (B) | % reduction environmental impact A relative to B |
|---|---|---|---|---|
| Climate change | kg $CO_2$ eq | 6.18E+00 | 3.42E+00 | 44.6 |
| Ozone depletion | kg CFC-11 eq | 4.53E−07 | 2.36E−07 | 47.9 |
| Human toxicity | kg 1,4-DB eq | 6.33E+00 | 5.32E+00 | 16.1 |
| Photochemical oxidant formation | kg NMVOC | 9.81E−03 | 5.54E−03 | 43.5 |
| Particulate matter formation | kg PM10 eq | 4.12E-03 | 1.21E-03 | 70.7 |
| Ionising radiation | kg U235 eq | 6.93E−01 | 6.24E−01 | 9.9 |
| Terrestrial acidification | kg SO2 eq | 1.35E−02 | 2.13E−03 | 84.3 |
| Freshwater eutrophication | kg P eq | 6.26E−06 | −7.82E−06 | 225.0 |
| Marine eutrophication | kg N eq | 3.44E−03 | 2.03E−03 | 40.9 |
| Terrestrial ecotoxicity | kg 1,4-DB eq | 9.22E−04 | 1.17E−03 | −27.1 |
| Freshwater ecotoxicity | kg 1,4-DB eq | 5.81E−04 | 4.61E−03 | −693.4 |
| Marine ecotoxicity | kg 1,4-DB eq | 2.19E+00 | 6.31E+00 | −188.4 |
| Agricultural land occupation | $m^2a$ | 1.23E−03 | 6.47E−02 | −5180.9 |
| Urban land occupation | $m^2a$ | 1.33E−04 | 7.71E−03 | −5690.0 |
| Natural land transformation | $m^2$ | 3.60E−06 | 3.67E−04 | −10114.0 |
| Water depletion | $m^3$ | 8.04E−01 | 2.95E−02 | 96.3 |
| Metal depletion | kg Fe eq | 8.22E−03 | 8.23E−02 | −901.2 |
| Fossil depletion | kg oil eq | 2.94E+00 | 2.22E+00 | 24,5 |

(Morales-Mora et al. 2012a), it was discussed that the metals that are not present in this case have a strong influence in modeling human toxicity (Dreyer et al. 2003), distorting the results obtained. Therefore, it is recommended the use of the specific models like USEtox™ model (Rosenbaum et al. 2008) to predict a potential increase in morbidity of workers or local human population per unit of chemicals released by the petrochemical industry.

### *3.1.2 Vinyl chloride monomer case study*

In the case of the VCM, both scenarios differ from each other because they present different ability, technological changes, generation of by-products, and waste. According to Table 5, both showed reductions of 50 % in different impact categories, but in others, they increased in the same proportion. The results obtained in the scenario B, phase of operation (ex post), have an increase of 50 % of adverse environmental impacts in comparison to scenario A, especially in categories related to the effect of the substances to human health and toxicity to ecosystems.

From the viewpoint of the process, the main cause of such impacts was the fact that the plant operated (scenario B) initially at a service factor below 30 % of the capacity, increasing the negative environmental impacts related to energy, water and raw materials consumption, and generation of chlorinated organic at higher concentrations than the originally specified. Due to this fact, the effluent from the process, recorded high concentrations of 1,2-dichloroethane and polycyclic aromatics. Moreover, in some sections of the plant the old equipment was not renewed. Table 6 shows the end-point categories evaluation. Thus, there was a total increase of 41.61 % in the damage category in scenario B, with the resources-availability impact category comprising the highest contribution. In general, these findings are consistent with previous LCA studies for VCM (PE-EuropeGmbH 2004) and studies on the health of workers occupationally exposed to VCM (Scléo et al. 2004; Gennaro et al. 2008).

In this regard, the modeling of mid- and end-points categories matches (empirical evidence) with the term "chain of causality" that describes the sequence of environmental mechanisms, which causes a particular issue and at the end it has an environmental damage (Potting and Hauschild 2005).

**Table. 6** Increasing percent of IA between ex post situation of the project and the redesign

| Category of damage (ReCiPe) | Unit | VCM redesign Scenario (A) | VCM ex post Scenario (B) | % reduction environmental impact B relative to A |
|---|---|---|---|---|
| Total | Pt | 0.558 | 0.956 | 41.61 |
| Human health | Pt | 0.201 | 0.258 | 22.04 |
| Ecosystems | Pt | 0.020 | 0.026 | 21.91 |
| Resources | Pt | 0.337 | 0.672 | 49.90 |

**Table. 5** Percentage change of the environmental impacts in midpoint categories in the VCM plant at A and B scenarios

| Impactcategory | Unit | VCM 2004 (scenario A) | VCM 2009 (scenario B) | % change of environmental impact B vs A |
|---|---|---|---|---|
| Climate change | kg $CO_2$eq | 5.40E+00 | 6.85E+00 | 21.2 |
| Ozone depletion | kg CFC-11 eq | 2.23E−06 | 2.94E−06 | 24.1 |
| Human toxicity | kg 1,4-DB eq | 7.67E−01 | 4.43E−01 | −73.2 |
| Photo-chemical oxidant formation | kg NMVOC | 6.44E−03 | 1.58E−02 | 59.3 |
| Particulate matter formation | kg PM10 eq | 3.36E−03 | 6.21E−03 | 45.9 |
| Ionizing radiation | kg U235 eq | 1.27E+00 | 1.12E+00 | −13.1 |
| Terrestrial acidification | kg $SO_2$eq | 1.00E−02 | 1.96E−02 | 48.9 |
| Freshwater eutrophication | kg P eq | 1.16E−04 | 6.00E−05 | −92.9 |
| Marine eutrophication | kg N eq | 2.11E−03 | 4.86E−03 | 56.6 |
| Terrestrial ecotoxicity | kg 1,4-DB eq | 6.90E−04 | 4.75E−04 | −45.3 |
| Freshwater ecotoxicity | kg 1,4-DB eq | 5.20E−03 | 4.47E−03 | −16.3 |
| Marine ecotoxicity | kg 1,4-DB eq | 9.54E−03 | 5.74E−03 | −66.3 |
| Agricultural land occupation | $m^2a$ | 2.96E−02 | 1.87E−02 | −57.9 |
| Urban land occupation | $m^2a$ | 7.35E−03 | 6.24E−03 | −17.8 |
| Natural land transformation | $m^2$ | 1.64E−04 | 6.92E−04 | 76.2 |
| Water depletion | $m^3$ | 3.85E−01 | 1.04E+00 | 63.1 |
| Metal depletion | kg Fe eq | 1.00E−01 | 5.23E−02 | −92.3 |
| Fossil depletion | kg oil eq | 1.53E+00 | 3.05E+00 | 49.8 |

**Table 7** Comparison reference marginal prevention costs of acrylonitrile from eco-costs database vs. Morelos acrylonitrile (eco-costs adjusted for Mexico)

| Unit (kg) | Total eco-costs (USD) | Global warming potential 100 (USD) | Acidification (USD) | Eutrophication (USD) | Summer smog (USD) | Fine Dust (PM 2.5) (USD) | Aquatic ecotoxicity (USD) | Carcinogens (USD) | Metals Depletion |
|---|---|---|---|---|---|---|---|---|---|
| Acrylonitrile [a] (eco-costs database) | 1.065 | 0.740 | 0.201 | 0.043 | 0.003 | 0.020 | 0.023 | 0.002 | 0.033 |
| Acrylonitrile old design[b] (A) | 1.623 | 1.595 | 0.0003 | 0.000 | 0.000 | 0.022 | 0.002 | 0.001 | 0.003 |
| Acrylonitrile redesign[c] (B) | 0.926 | 0.853 | 0.018 | 0.000 | 0.002 | 0.007 | 0.016 | 0.001 | 0.030 |

[a] http://www.ecocostsvalue.com/index.html

[b,c] Own estimate for Mexico

## 3.2 Economic analysis: linking LCIA-Eco-costs, NPV and IRR

### *3.2.1 Acrylonitrile case study*

The results of the LCIA (mid-point categories) were combined with the eco-costs database. Then, the eco-costs for both scenarios were calculated by linear interpolation from the results of the LCIA and were compared with eco-costs database to obtain the eco-costs adjustment for Mexico (phase III of the Fig. 4) by the eight impact category and total eco-costs (Table 7). These values are different from the ones reported by Morales-Mora et al. (2012a) because they had not incorporated the methodological improvement (i.e., eco-costs adjusted for Mexico).

Table 7 showed that total eco-costs were 1.065 USD/kg for acrylonitrile database and 0.926 USD/kg for the Morelos Complex Acrylonitrile redesign. However, in this plant, the

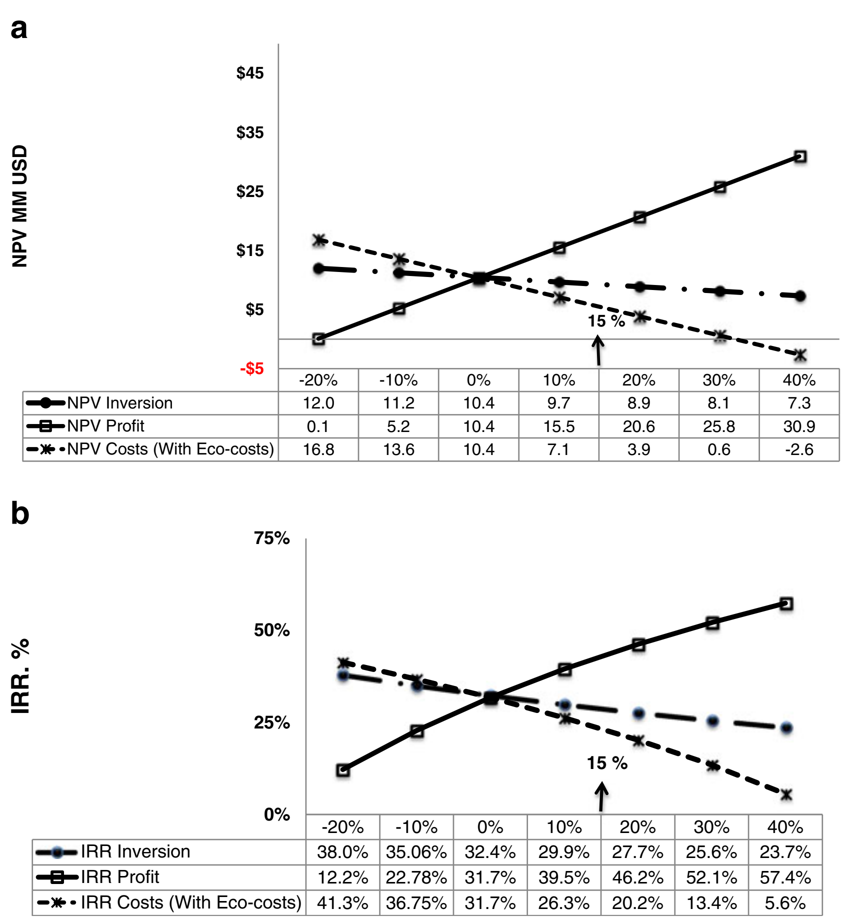



**Fig. 5** Sensitivity analysis for the acrylonitrile project: **a** NPV and **b** IRR with 15 % of eco-costs, obtained through LCIA

**Table 8** IRR and NPV results obtained by the proposed methodology

| Process | Total eco-costs (norms for sustainability) USD/kg | Price of products USD/kg[b] | Adjustment eco-costs (current methodology (%) | IRR % | NPV (social-environmental) USD millions |
|---|---|---|---|---|---|
| Acrylonitrile (eco-costs database)[a] | 1.065 | | | | |
| Acrylonitrile old design (scenario A) | 1.623 | | | | |
| Acrylonitrile redesign (scenario B) | 0.926 | 1.65–2.3 | 15 | 24.0 | 5.89 |

[a] http://www.ecocostsvalue.com/index.html

[b] PEMEX-PETROQUIMICA (price adjusted according to FU)

virtual eco-costs to prevent the environmental impacts and resources depletion comprises about 40–56 % of the market price. In order to find the eco-costs percentage which allows the profitability and viability of the project a sensitivity analysis was carried out. Its results are shown in Fig. 5. Hence, Fig. 5a shows that if eco-costs increase, NPV decreases. Without any increase, NPV is 10.4 million USD, but with an increase of 10 % in costs, NPV decreases 7.1 million USD. If cost increases 20 %, NPV decrease to 3.9 million USD, and 40 %, NPV is negative. It is evident that, without any increase, the IRR is 31.7 %, and as the eco-costs increase, the IRR decreases. In conclusion, the project supports (i.e., feasible project) an increase in eco-costs with NPV and IRR values between 10 and 15 %.

Although an adequate IRR of 24 % and a NPV of 5.89 million USD are obtained, the project is viable in terms of private profitability. The advantage of these results is that, by this methodology, the social costs (environmental) are incorporated (Table 8).

### 3.2.2 Vinyl chloride monomer case study

Table 9 presents the comparison of eco-costs for both scenarios, evaluated with the VCM eco-costs database (Vogtländer et al. 2010).

Scenario A (VCM redesign) recorded 16.08 USD/kg of VCM, being the highest value, mainly because the negative impact of the acidification impact category is about 90 % of the total eco-costs. In scenario B, the total eco-costs was 1.62 USD/kg of VCM, and the highest impact was produced by acidification as well, comprising about 51 % of the total of the eco-costs. However, the principal issues of the VCM process are the health impact by the dioxins formed during the production of EDC by oxychlorination (PE-EuropeGmbH 2004; UNEP 2005) and by the increased risk of lung cancer in workers occupationally exposed to VCM (Scléo et al. 2004; Gennaro et al. 2008).

Comparing the three cases, the benchmarking case VCM Ecoinvent from EU, was only 0.476 USD/kg of VCM, which is 34 times lower than the value calculated in scenario A and 3.46 times lower than that one calculated for case B.

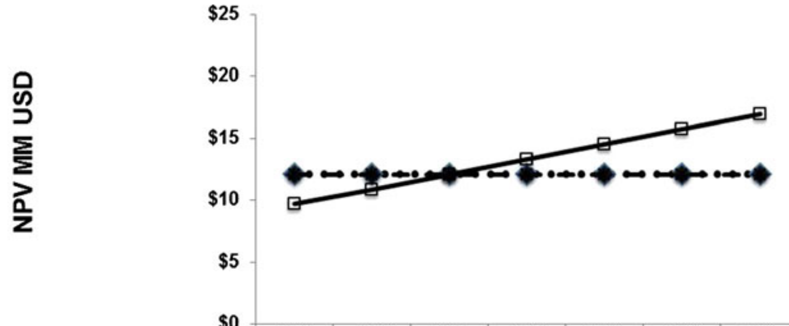
Furthermore, the virtual eco-costs to prevent the environmental impacts and resources depletion for the VCM is more than the 100 % of the sale price for scenario B (ex post), and 50 % higher than the benchmarking case. Thus, it is not viable to incorporate them when considering the private return. In this case, the sensitivity analysis allowed evaluating the effect of initial investment and benefits and costs in the VCM project. It was found that 1.5 % of the eco-costs (Fig. 6) can be integrated into the project as private profitability, which is an adequate yield with an IRR of 11.7 % and an NPV of 7.65 million USD, making it thus a financially viable project (Blank et al. 2005).

**Table 9** Comparison reference marginal prevention costs of VCM wco-costs data base vs. Pajaritos VCM study (adjusted for Mexico)

| Unit (kg) | Total eco-costs (USD) | Global warming potential (USD) | Acidification (USD) | Eutrophication (USD) | Summer smog (USD) | Fine dust (PM 2.5) (USD) | Aquatic ecotoxicity (USD) | Carcinogens (USD) | Metals depletion (USD) |
|---|---|---|---|---|---|---|---|---|---|
| VCM (eco-costs database)[a] | 0.476 | 0.000 | 0.060 | 0.001 | 0.002 | 0.005 | 0.017 | 0.000 | 0.002 |
| VCM (scenario A)[b] | 16.088 | 0.847 | 14.486 | 0.00 | 0.033 | 0.668 | 0.024 | 0 | 0.0314 |
| VCM (scenario B)[c] | 1.621 | 1.016 | 0.522 | 0.00 | 0.008 | 0.035 | 0.016 | 0 | 0.0232 |

[a] http://www.ecocostsvalue.com/index.html

[b,c] Own estimate for Mexico




| | -20% | -10% | 0% | 10% | 20% | 30% | 40% |
|---|---|---|---|---|---|---|---|
| NPV Inversion | 12.1 | 12.1 | 12.1 | 12.1 | 12.1 | 12.1 | 12.1 |
| NPV Profit | 9.7 | 10.9 | 12.1 | 13.3 | 14.5 | 15.7 | 16.9 |
| NPV Costs (With Eco-costs) | 12.1 | 12.1 | 12.1 | 12.1 | 12.1 | 12.1 | 12.1 |

**Fig. 6** Sensitivity analysis for the VCM project

As shown in both scenarios, the estimation of the virtual eco-costs to prevent the environmental impacts and resources depletion gives an important tool for improving and selecting the most adequate technology to reach the best practice in both pollution control and prevention in the design (or conceptual engineering) phase. Therefore, the co-products, energy consumption, and generation of hazardous waste at the first phase of the development of the project can be optimized (Korpi and Ala-Risku 2008).

## 3.3 Sensitivity analysis of environmental performance

### 3.3.1 Acrylonitrile case study

The results of sensitivity analysis according to Monte Carlo methods performed for each impact category of the two alternatives analyzed (old design vs. redesign of the acrylonitrile plant) are reported by Morales-Mora et al. (2012a).

### 3.3.2 Vinyl chloride monomer case study

In Fig. 7, the results of the sensitivity analysis for both scenarios are shown. The green bars on the left represent the times that the environmental burden is lower in scenario A (redesign) than in scenario B. Clearly, the sensitivity analysis confirmed that there is no uncertainty about the inventory data when measurements are performed in the laboratory of the plant from direct samples taken during the process. This may be due to the fact that scenario A presented a reduction in the environmental impacts, due to the increase in the plant production capacity. In scenario B (ex post), the results are consistent with the results obtained in Table 5, since negative impacts were recorded in the same impact categories: atmosphere, soil, and water emissions and fossil fuels consumption. Therefore, there is a high precision degree of the impact category results obtained for both scenarios, which define the uncertainty based on three parameters (Frischknecht et al.

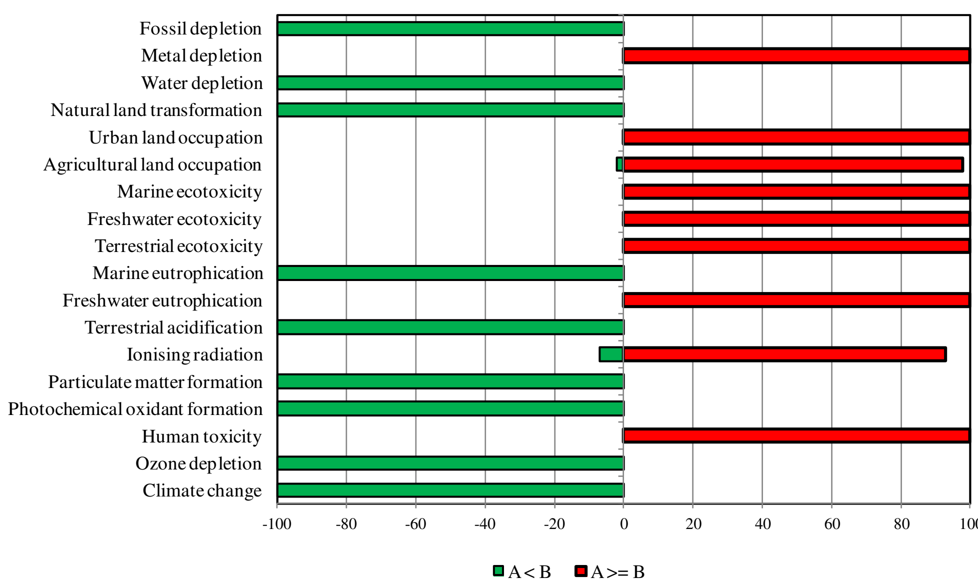



**Fig. 7** Results of the comparison of Monte Carlo analysis in different categories of impact of scenarios A and B to the VCM process

2007): reliability, temporality, and geography. In the case of VCM, the uncertainty factor is 1.0, which is the lowest of the five proposed levels.

## 4 Conclusions

The improvements proposed in the methodology provided the adjustment of prices of the database of eco-costs determined for Western Europe and its adaptation to economic conditions of Mexico through benefit transfer. In addition, it was possible to incorporate the potential environmental impacts through the marginal prevention costs by LCA to financial analysis of projects for two petrochemical processes.

This integrated methodology takes into account the amount of environmental burden of petrochemical products and their costs, which should reduce the environmental pollution and material depletion. However, these eco-costs comprise in the acrylonitrile case, 40–56 % the selling price of the product, and more than 100 % for the VCM case. Therefore, the sensitivity analysis, through variation in investment, benefits, and costs (eco-costs) to the NPV and IRR, identified how much of this eco-costs could be incorporated into the project to make it profitable. Values above a range between 10 and 15 % to these materials would make it impractical and therefore the financial project would be rejected.

These tools might have practical applications such as: (1) assessing the profitability of a project, (2) to value the services provided by the country's natural capital, (3) to offset the high costs of green net national product, and (4) to establish investment strategies, like reducing the pollution at source from the design stage of a project, linking the value chain to the ecological product chain. Thus, this methodology provides a clear mechanism based on LCA that shows how to incorporate the environmental burden that generates a product, process or service to monetary units to the decision making to accept or reject a project, from the perspective of private profitability but with a clear sustainability focus.

Finally, in spite that the BT method is put into question by a number of economists, it has proven useful for environmental services valuation (e.g., Wilson and Hoehn 2006) and for integrating LCA with life cycle costing (Manmek 2007). We recognize that our approach is a valid benchmark, which contributes to the assessment of eco-costs in important industries, such as that of petrochemicals in emerging economies. Otherwise, analyses in such countries would be even scarcer. Yet, we reckon that developing countries should put more efforts in estimating local eco-costs for having more accurate assessments.

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